Field enhancement and saturation of millimeter waves inside a metallic nanogap

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Abstract: This paper investigates the millimeter electromagnetic waves passing through a metal nanogap. Based upon the study of a perfect electrical conductor model, we show that the electric field enhancement inside the gap saturates as the gap size approaches zero, and the ultimate enhancement strength is inversely proportional to the thickness of the metal film. In addition, no significant enhancement can be gained by decreasing the gap size further if the aspect ratio between the dimensions of the underlying geometric structure exceeds approximately 100.

OCIS codes: (310.6628) Subwavelength structures, nanostructures; (050.6624) Subwavelength structures (240.3695); Linear and nonlinear light scattering from surfaces; (350.4238) Nanophotonics and photonic crystals.

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1. Introduction

The extraordinary optical transmission effect through subwavelength apertures (see [1]) has been extensively investigated in recent years, both theoretically and experimentally, due in part to its significant potential applications in sensing, spectroscopy, and nano-optics. When an electromagnetic wave impinges upon a metallic gap, it has been shown experimentally that the electric field enhancement keeps increasing with a decreasing gap width that ranges from micrometers to nanometers [2–13]. A natural question arises for such field enhancement: if the gap size keeps decreasing, will the electric field finally saturate in the classical regime?

It has been explored that there is limiting behavior for the field enhancement in nanogap structures due to the mechanism of nonlocality and quantum mechanical tunneling [14, 15]. Here we show, rather surprisingly, that even in the absence of these effects and assuming a perfect electrical conductor, the field enhancement will be limited by a purely geometrical effect for millimeter electromagnetic waves. It is demonstrated that the electric field enhancement remains bounded as the gap size goes to 0, and the upper limit of the field amplitude strength is inversely proportional to the thickness of the metal film. In addition, the field enhancement saturates when the aspect ratio between the metal thickness and the gap width reaches approximately 100. A mathematical theory is described in this paper, and various numerical simulations based upon the solution of the mathematical model are demonstrated to validate our claims.

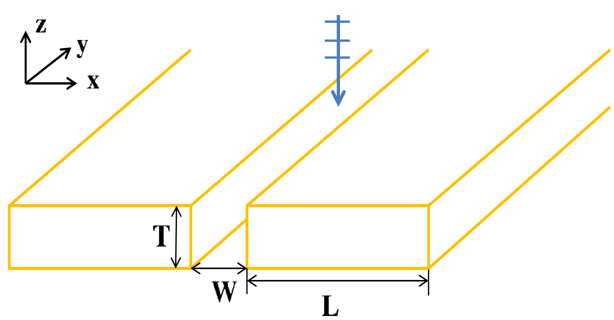

Fig. 1. Geometry of the problem.

Consider a polarized monochromatic wave that impinges normally upon the metal films (see. Fig. 1). The magnetic field vector is parallel to the y direction such that the incident wave $H^{inc} = (0, e^{-ikz}, 0)$, wherein k is the wavenumber. A single long slit is formed by two identical

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metal films that have infinite length along the y direction, the width L and the thickness T as shown in Fig. 1. The slit is infinite in the y direction, and it forms a gap aperture on the xy plane with a width of W. We are interested in the electric field enhancement when the length scale of the underlying geometry is given by $L/\lambda \sim 1$ and $W/\lambda << T/\lambda << 1$. Here λ represents the wavelength of the incident wave, which is in the millimeter regime. In particular, if $W/\lambda \sim 10^{-6}$, the aperture of the slit becomes a nanogap.

Here and thereafter, we restrict our discussion to the xz plane since the problem under consideration is the transverse magnetic (TM) polarized case. In this way, the slit under consideration is reduced to a rectangle on the xz plane. The standard Cartesian coordinate system is adopted such that the origin corresponds to the lower left corner of the slit.

The electromagnetic wave after scattering consists of the scattered wave and the incident wave. The y component of the magnetic field H_y satisfies the Helmholtz equation outside the metal region on the xz plane:

$$\frac{\partial^2 H_y}{\partial x^2} + \frac{\partial^2 H_y}{\partial z^2} + k^2 H_y = 0. \tag{1}$$

In the millimeter wave regime, we can assume that the metal is a perfect electrical conductor (PEC). Hence the normal derivative

$$\frac{\partial H_y}{\partial n} = 0 \quad \text{on the metal boundaries.} \tag{2}$$

In addition, at infinity the scattered wave satisfies the Sommerfeld radiation condition [16].

2. Electric field enhancement inside the nanoslit

Let E be the total electric field, which consists of the incident wave E^{inc} and the induced field, then the electric field enhancement factor for a given slit is defined by

$$Q = \frac{\int_{\text{slit region}} |E| \, dxdz}{\int_{\text{slit region}} |E^{inc}| \, dxdz}.$$

Using the fact that $|E^{inc}|$ is invariant in the slit region, it yields that

$$Q = \frac{1}{A} \int_{\text{slit region}} \frac{|E|}{|E^{inc}|} \, dxdz, \tag{3}$$

where A is the area of the slit region.

For a length scale with $L/\lambda \sim 1$ and $W/\lambda << T/\lambda << 1$, the magnetic field H_y, which is the solution of governing Eqs. (1)–(2), admits an asymptotic expansion in terms of the small parameters T and W. We direct the readers to [18] for the detailed rigorous derivation of the asymptotic expansion formula. Briefly speaking, it is shown that, H_y is almost a linear function inside the slit, and it is close to the field value in the absence the slit above and below the metal films. Based on the asymptotic expansion formula, it is proved that the electric enhancement factor is of the order $O(\frac{1}{Tk})$ and does not blow up even if the gap width keeps decreasing. The readers are refer to [18] for a mathematical proof of this statement. We point out that, due to the scaling invariance of the Maxwell equations, such enhancement behavior remains true in other electromagnetic frequency regimes, such as terahertz or megahertz waves, as long as the length scale reaches a threshold such that $W/\lambda << T/\lambda << 1$ and the width of the metal film L is at least comparable to the wavelength λ.

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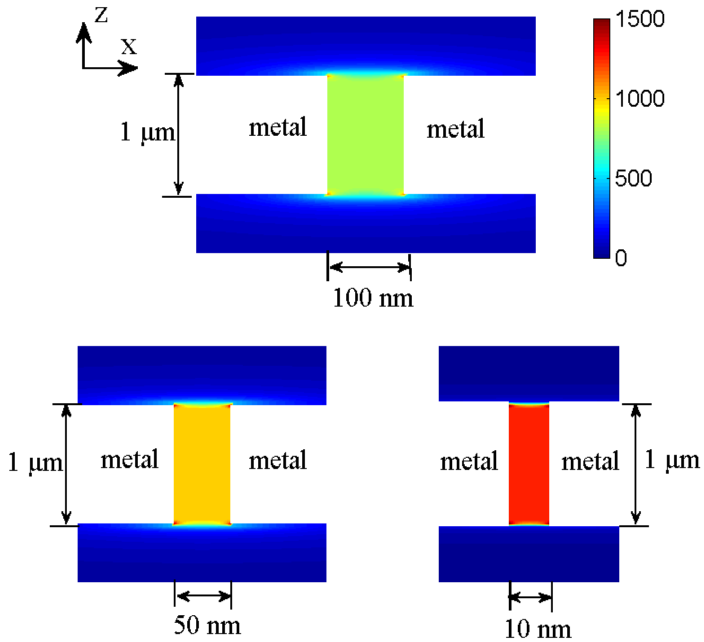

Fig. 2. Electric field enhancement $|E|/|E^{inc}|$ inside and near the nano slit when the gap width W is 100 nm, 50 nm, and 10 nm, respectively.

In the following, we illustrate the saturation behavior of the electric field from a numerical perspective. First, let us consider the configuration where the width and the thickness of the metal film is 6 mm and 1 μm, respectively. The frequency of the incident wave is 0.05 THz such that the wavelength $\lambda = 6$ mm. The magnetic field is obtained by solving Eqs.(1)–(2) with high-order accuracy via a boundary element method [17]. An adaptive strategy is employed to evaluate the associated integrals in a fast and accurate manner.

Figure 2 shows the pointwise electric field enhancement $|E|/|E^{inc}|$ in the slit when the gap width W is 100 nm, 50 nm, and 10 nm, respectively. The enhancement factor Q is approximately 809, 1000, 1260 respectively for the three gaps considered. It is observed from the figure that $|E|/|E^{inc}|$ is almost invariant in the slit except in the regions near the gap apertures. Indeed, this significant property is attributed to the linearity of the magnetic field inside the slit. To illustrate this phenomenon, Fig. 3(a) plots the magnetic field H_y on the xz plane in the slit region for $W = 100$ nm. For clarity, Fig. 3(b) demonstrates the value of H_y in the middle of slit along the z direction, and Fig. 3(c) is the value of H_y on the horizontal cross-sectional lines of the slit. It is observed that, away from gap apertures, H_y is linear inside the slit along the z direction and invariant along the x direction. Analytically, the wave field inside the slit can be expanded as the sum of wave-guide modes [11, 18]:

$$H_y(x,z) = \sum_{n=0}^{\infty} \left(\alpha_n e^{i\gamma_n z} + \beta_n e^{-i\gamma_n (z-T)} \right) \cos\left(\frac{n\pi x}{W}\right), \tag{4}$$

wherein $\gamma_n = \sqrt{k^2 - (n\pi/W)^2}$. Since $W/\lambda << 1$, it is apparent that the modes $e^{i\gamma_n z} \cos\left(\frac{n\pi x}{W}\right)$ and $e^{-i\gamma_n (z-T)} \cos\left(\frac{n\pi x}{W}\right)$ decay exponentially away from the lower and upper gap apertures

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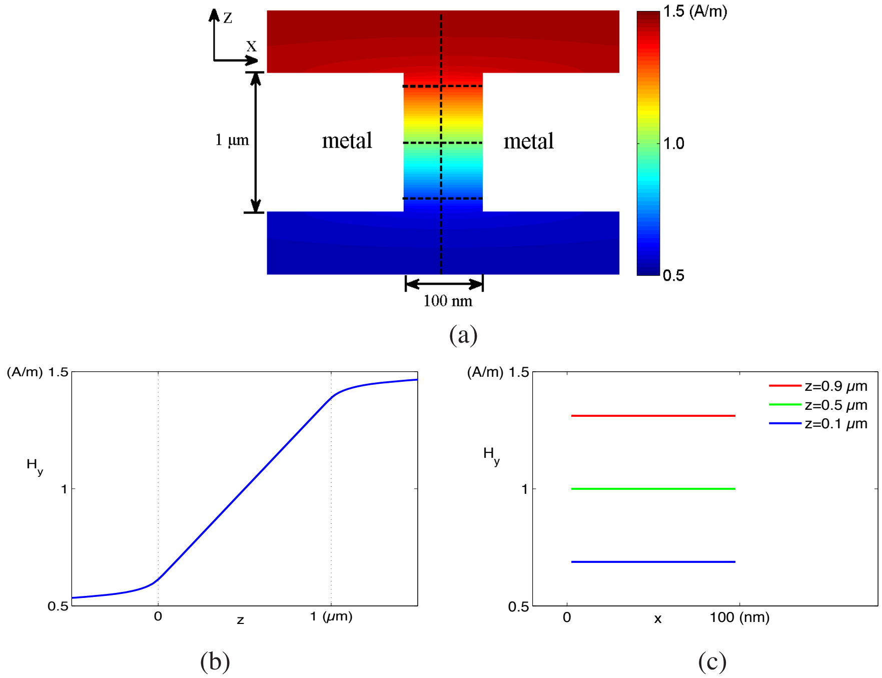

Fig. 3. (a). Magnetic field H_y inside and near the nano slit; (b). H_y in the middle of slit along the z direction (vertical dash line in (a)); (c). H_y on the cross-sectional lines of the slit (horizontal dash lines in (a)).

respectively with a rate of $O(e^{-n/W})$ for all $n \geq 1$. On the other hand, by a simple calculation, the lowest mode with $n = 0$ can be recast as

$$B_1 \sin(kz + \phi_1) + i\, B_2 \sin(kz + \phi_2). \tag{5}$$

Here B_1 and B_2 are the amplitudes which are of order $O(\lambda/T)$, and ϕ_1 and ϕ_2 are the phase shifts. Using the fact that $T/\lambda << 1$, a Taylor expansion gives

$$\sin(kz + \phi_i) = \sin\phi_i + 2\pi\cos\phi_i \cdot (z/\lambda) + O(z^2/\lambda^2), \quad i = 1, 2. \tag{6}$$

By virtue of (4)–(6), it can be assumed that the magnetic field is a linear function represented by

$$H_y(x,z) = az + b \quad \text{for } \delta \leq z \leq T - \delta, \tag{7}$$

where δ is a negligibly small number compared to the metal thickness T. From (7) and the Ampere's law $\nabla \times H = -i\omega\varepsilon E$, we see that, inside the slit, the electric field

$$E = (E_x, 0, 0) \qquad \delta \leq z \leq T - \delta,$$

and the x component of the electric field $E_x = \dfrac{a}{i\omega\varepsilon}$. Thus by noting that $|E^{inc}| = \frac{k}{\omega\varepsilon}$, the resulting piecewise enhancement factor becomes

$$\frac{|E|}{|E^{inc}|} = \frac{|a|}{k}, \qquad \delta \leq z \leq T - \delta. \tag{8}$$

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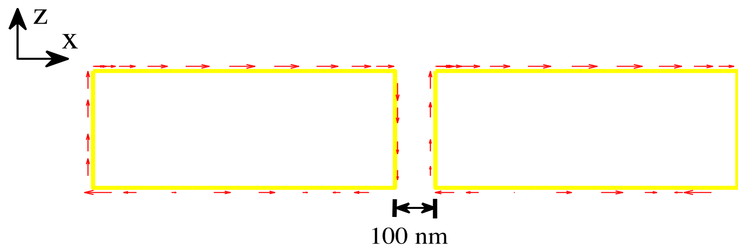

Fig. 4. The induced current on the surface of metal films.

This explains why $|E|/|E^{inc}|$ is almost invariant in the slit, since both a and k in (8) are independent of x and z.

Let $a_{+,W}$ and $a_{-,W}$ be the values of H_y on the upper and lower gaps respectively, wherein the subscript is used to denote their dependence on the gap size. From (8) and by noting that the slope a in (7) can be approximated by $(a_{+,W} - a_{-,W})/T$, the calculation of the electric field enhancement factor Q in (3) is simplified as

$$Q \approx \frac{|a_{+,W} - a_{-,W}|}{Tk}, \tag{9}$$

since δ is a negligibly small number compared to the thickness T. We immediately obtain that the enhancement factor is inversely proportional to the metal thickness T.

By solving the Helmholtz equation (1) with the boundary condition (2), the induced current $n \times H$ on the surface of the metal films can also be obtained. Figure 4 demonstrates the induced surface current for the gap width $W = 100$ nm.

3. Saturation of the enhancement with decreasing gap sizes

In order to investigate the ultimate field enhancement, we explore the change of the enhancement factor as the gap width decreases from 100 nm to a few nanometers. To obtain Q, we first examine $a_{+,W}$ and $a_{-,W}$ in (9), i.e., the values of H_y on the upper and lower gaps. Figure 5 demonstrates the magnetic field H_y along the boundaries of metal films for the gap size that ranges from 100 nm to 2 nm. For comparison, the magnetic field $H_{y,0}$ on the metal boundary is also shown for the case when no slit is present. It is observed that, as W decreases, along the outer boundaries of metal films (excluding the slit boundaries), the magnetic field H_y converges to $H_{y,0}$ eventually. In particular, at the gap apertures, the field values approach the no-slit field $H_{y,0}$ with decreasing gap sizes. To better illustrate such convergence behavior, we plot the magnetic field along the z direction in the middle of the slit in Fig. 6. It is apparent that the slope of the linear magnetic field increases steadily as the gap width decreases. In addition, the magnetic field values at upper and lower gaps, $a_{+,W}$ and $a_{-,W}$, eventually approach the upper and lower boundary values of $H_{y,0}$, $a_{+,0}$ and $a_{-,0}$, respectively. This is consistent with the mathematical theory described in [18]. Consequently, it is concluded that the enhancement factor Q saturates and finally approaches the limit value

$$Q_0 = \frac{|a_{+,0} - a_{-,0}|}{Tk}$$

as the gap width keeps decreasing. This is demonstrated in Fig. 7, where the enhancement factor Q for $W = 100$ nm, 50 nm, 10 nm, 5 nm, and 2 nm are obtained by solving the Helmholtz equation directly and applying the Ampere's law.

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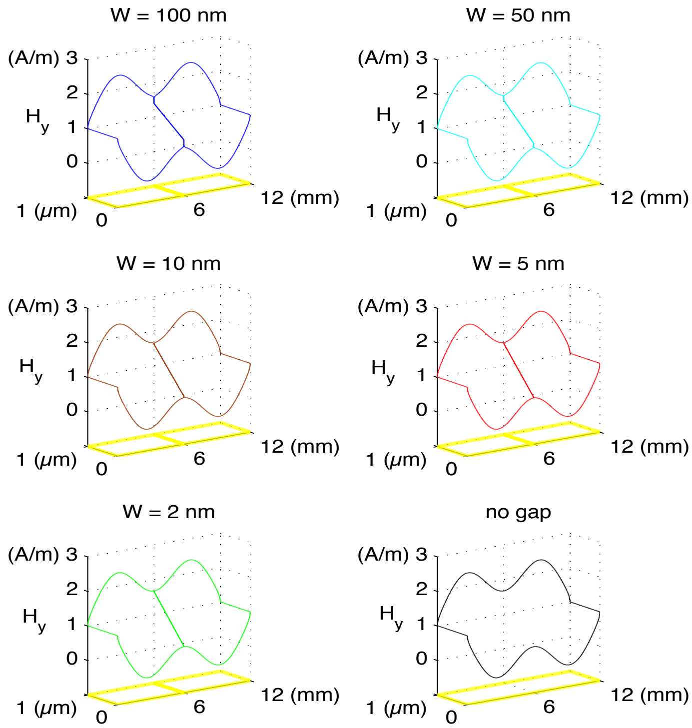

Fig. 5. Magnetic field H_y along the boundaries of metal films for gap width $W = 100$ nm, 50 nm, 10 nm, 5 nm, 2 nm, and the magnetic field $H_{y,0}$ when no gap is present. Note the change of field near the gap apertures when the gap size decreases.

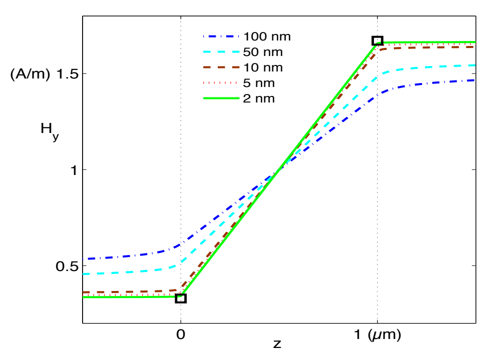

Fig. 6. Magnetic field H_y in the middle of the slit along the z direction for gap width $W =$ 100 nm, 50 nm, 10 nm, 5 nm and 2 nm, respectively. The black squares denote $a_{-,0}$ and $a_{+,0}$, the values of the magnetic field $H_{y,0}$ at $z = 0$ μm and $z = 1$ μm respectively in the absence of nano silt.

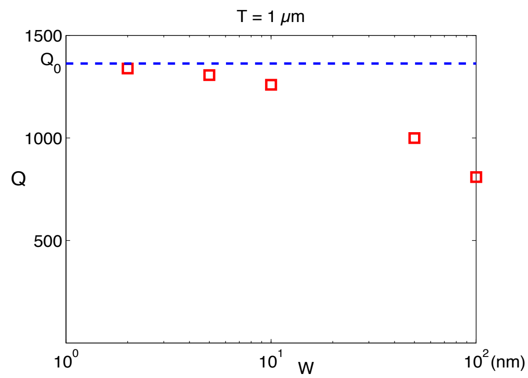

Fig. 7. Enhancement factor Q for gap width $W = 100$ nm, 50 nm, 10 nm, 5 nm and 2 nm, respectively. The metal thickness $T = 1$ μm. Q saturates and approaches the limit $Q_0 = \dfrac{|a_{+,0} - a_{-,0}|}{Tk}$ as the gap width decreases.

Let us set $r = Q/Q_0$ as the ratio between the enhancement factor Q for a nanogap and the ultimate enhancement factor Q_0. We obtain that $r = 60\%, 73\%, 93\%, 96\%$ and 98% respectively for the above considered gap sizes. More specifically, for a gap width of 10 nm, the enhancement ratio is 93%, and no significant enhancement is gained by a further decrease of the gap width. Note that the thickness of the metal film under consideration is 1 μm. Therefore, we may say that the electric field enhancement is almost saturated when the aspect ratio between the thickness of the metal film and the gap width reaches a value of 100.

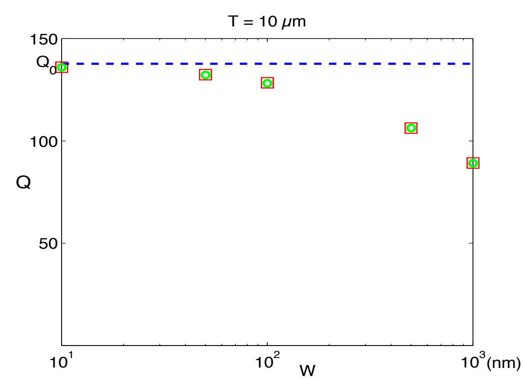

Fig. 8. Enhancement factor Q for gap size $W = 1\mu$m, 500 nm, 100 nm, 50 nm, and 10 nm, respectively. The metal thickness $T = 10$ μm. Square: calculation based on the PEC model; circle: calculation with the Drude model for real metals.

For a thick metal film with $T = 10$ μm, the convergence behavior of the electric field enhancement is demonstrated in Fig. 8 (the squares). The enhancement factor Q approaches the limit value $Q_0 \approx 137$ as W decreases. In particular, an enhancement ratio of 94% is achieved when $W = 100$ nm. To validate the PEC model, we compare the simulation results with real metals, in which the Drude model is employed to calculate the dielectric constant of the metal (gold) [19]:

$$\varepsilon(\omega) = 1 - \frac{w_p^2}{\omega(\omega + i\gamma)}.$$

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Here the plasma frequency $w_p = 1.37 \times 10^4$ THZ and $\gamma = 40.7$ THZ. The associated mathematical model for the nanogap is solved by the finite element method, and the enhancement factor Q is shown as the circles in Fig. 8. It is observed that the values obtained via the PEC and the Drude models are so close that their differences are indistinguishable from the figure.

4. Conclusion

This paper has investigated the electric field enhancement in the classical regime when the millimeter electromagnetic wave impinges upon a nanogap. It is shown that the electric field enhancement inside the nanoslit eventually approaches a finite value as the size of the gap aperture decreases. The ultimate enhancement factor is derived explicitly. In addition, we point out that such an enhancement almost saturates if the aspect ratio between the dimensions of the geometric structure reaches approximately 100.

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